Name: _____

PHYSICS 619 : SPRING SEMESTER 2019

**Project #10: PIMC and Langevin Algorithm**

1) Consider the following Hamiltonian for Hooke's atom

$$H = -\frac{1}{2}\nabla_1 - \frac{1}{2}\nabla_2 + \frac{1}{2}\mathbf{r}_1^2 + \frac{1}{2}\mathbf{r}_2^2 + \frac{\sqrt{2}}{|\mathbf{r}_2 - \mathbf{r}_2|}$$

   a) What is the second-order imaginary time propagator in this case?
   b) What is the local energy function in this case?
   c) Do a 2-, 4-, 6-propagator PIMC calculation to estimate its ground state energy. (5 pt bonus. What is the exact ground state energy?)

2) Use the Langevin Algorithm to do the variational Helium atom case with (in atomic units)

$$\Psi_T^2(r_1, r_2) = \mathrm{e}^{-2\alpha r_1}\mathrm{e}^{-2\alpha r_2}.$$

   at $\alpha = 1.6875$ and

$$H = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \frac{2}{r_1} - \frac{2}{r_2} + \frac{1}{r_{12}}.$$

   Choose a serie of time step sizes such as $\Delta t = 0.09, 0.07, 0.05, 0.04, 0.03, 0.02, 0.01$ etc., until you see the linear convergence.

3) Repeat the same calculation but now uses the Generalized Metropolis algorithm, which is the Langevin algorithm with an acceptance/rejection step. Verify that the result you get now is independent of $\Delta t$.

4) The Generalized Metropolis algorithm removed the step-size error by an additional acceptance/rejection step, which adds substantial overhead. To improve on the first-order Langevin algorithm, can you devise a second-order Langevin algorithm to reduce the step-size error dependence to $(\Delta t)^2$? Repeat 1) using this second-order Langevin algorithm.